Phosphoramidic acid, dimethyl-, dimethyl ester

597-07-9	DTXSID20208405	

Model Performance

Model	Data

Weighted KNN model

5-fold CV (5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.87	0.81	0.87	0.82	0.86	0.86	

Model Results

Predicted value: 2.05 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.45e-01

Confidence level: 6.65e-01

Nearest Neighbors from the Training Set

Image not found

Dimefox

Measured: 6.49 **Predicted:** 4.15

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Hexamethylphosphoramide

Measured: 5.58 Predicted: 3.41

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Trimethyl phosphate Measured: 3.57 Predicted: 3.64

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Ethyl dimethyl phosphate

Measured: 3.24 Predicted: 3.42